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Developing theoretical beamlines for local, ultrafast and magnetic-field induced spectroscopic effects

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The last two decades have witnessed enormous advances in synchrotron and laser technology, allowing for the detection of increasingly sophisticated light-matter interactions. To fully capitalize on the opportunities offered by these experimental advances, new theories, concepts and computational tools are mandatory, as they are essential to be able to interpret the experimental results and to retrieve precise quantitative chemical information.

During the talk, I will review some of our more recent efforts to develop highly reliable quantum chemical methods and computational protocols to model the response of molecular systems when probed with electromagnetic fields in new and challenging combinations. Specific examples are advanced (time-resolved) core-level spectroscopies [1,2,3,4,5,6,7], photoionization/photoelectron phenomena [8], and sophisticated magneto-optical effects [9,10,11]. Our ambition is to bridge experimental measurements and theory at a hitherto unprecedented level of detail and accuracy.

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